



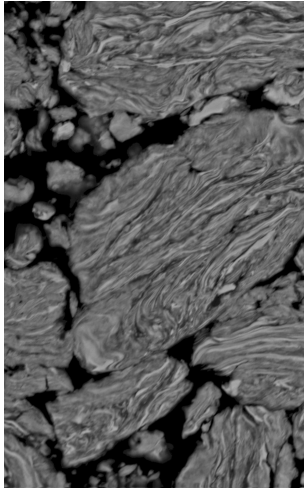
Center for Shock Wave-processing of Advanced Reactive Materials (C-SWARM)

Karel Matouš

Co-Director



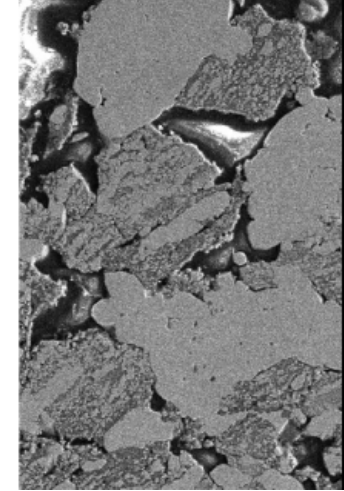
Shock Wave-processing of Advanced Reactive Materials



High Energy Ball
Milling (HEBM)



C-SWARM
Verification
Prediction



Validation/UQ
Discovery

- Continuum modeling framework
- Truly multiscale in space, time, and constitutive equations
- Chemo-thermo-mechanical behavior
- Solid-solid state transformations

Shock Wave-processing of Advanced Reactive Materials



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Computational
Physics

Notre Dame



A. Mukasyan



S. Paolucci

Computer
Science

Indiana/Notre Dame

V&V/UQ

Purdue/Notre Dame



J. Powers



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A. Lumsdaine



T. Sterling



S. Son

Shock Wave-processing of Advanced Reactive Materials

► Computational Physics

- Image-based Modeling
- Algorithms Development
- Scale-Time Bridging
- Constitutive Equations

► Experimental Physics, V&V/UQ

- Material Characterization
- Constitutive Model Calibration
- Validation Experiments
- Verification and UQ

- P-P-P Integration
- Educational Component
- C-SWARM Management
- Risk Mitigation

► Computer Science

- ParalleX Model
- HPX runtime system
- Advanced Libraries
- DSeL

► Software Plan

- Combines CP, CS & EP
- Mini-apps
- Software Engineering

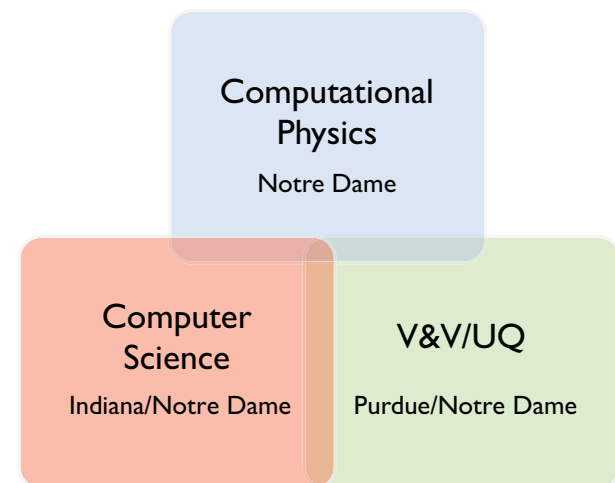
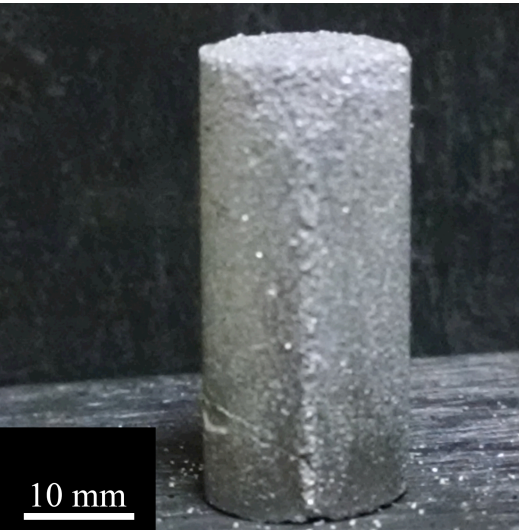
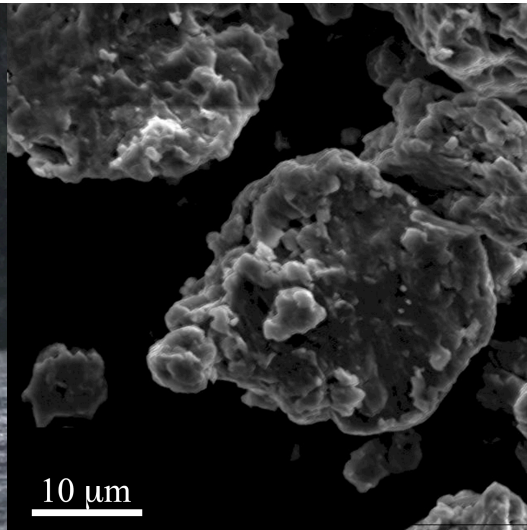


Image-Driven Modeling

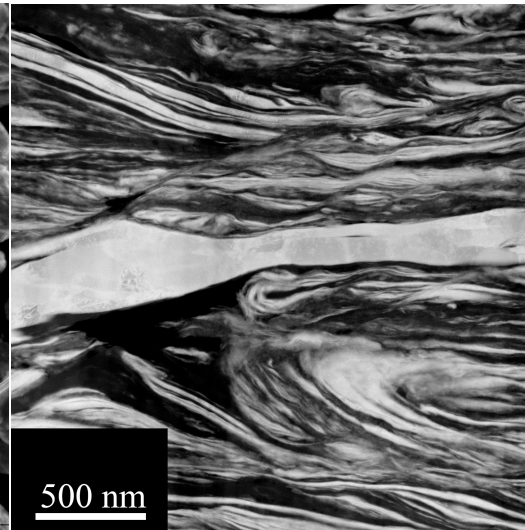
Macroscale



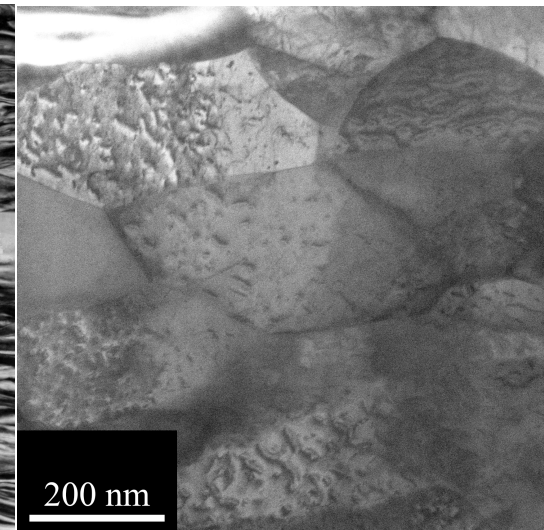
Mesoscale



Microscale



Nanoscale



■ Targeted Characteristics:

- Porosity
- Pellet Size and Shape

■ Targeted Characteristics:

- Particle Size
- Particle Shape

■ Targeted Characteristics:

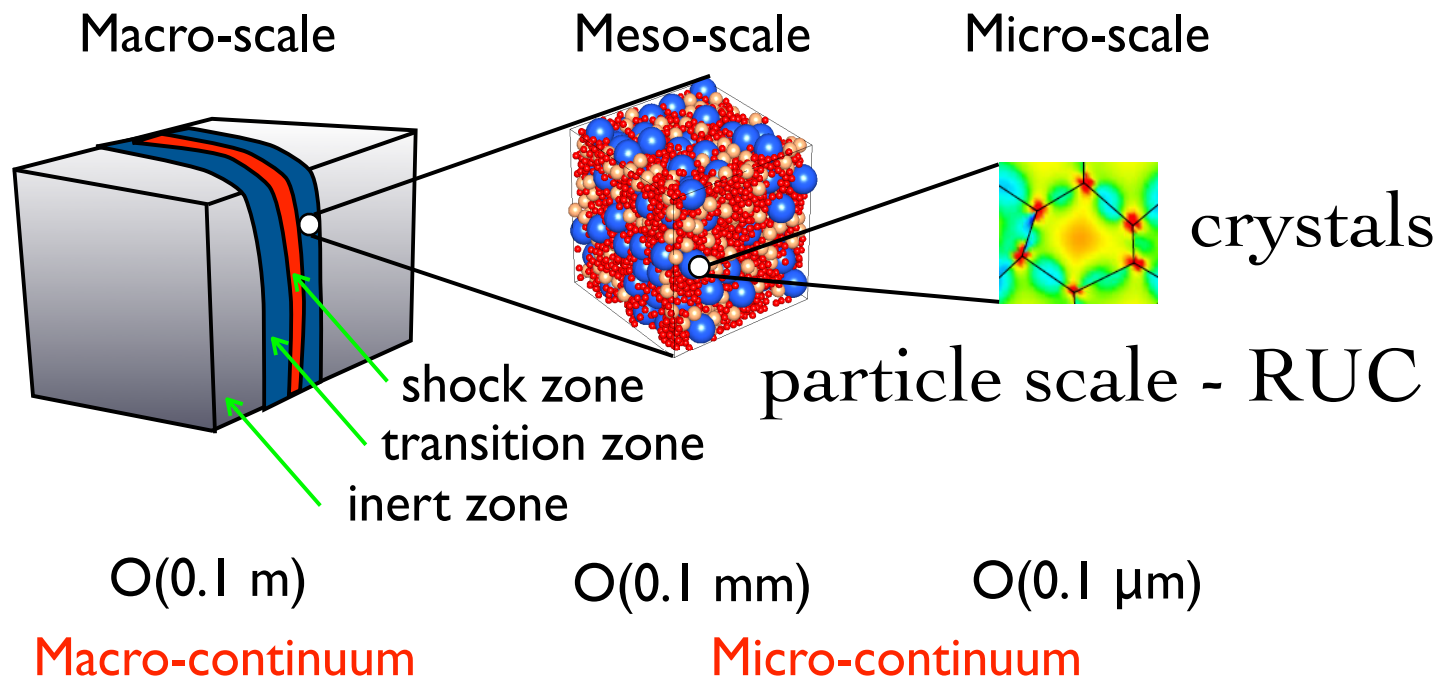
- Layer Thickness
- Layer Tortuosity
- Reactant Surface Area Contact

■ Targeted Characteristics:

- Crystal Size
- Crystal Shape
- Crystal Orientation

Modeling and Computational Aspects

- Hierarchical multiscale modeling concept
- Macro(M) and micro(m) codes - M&m



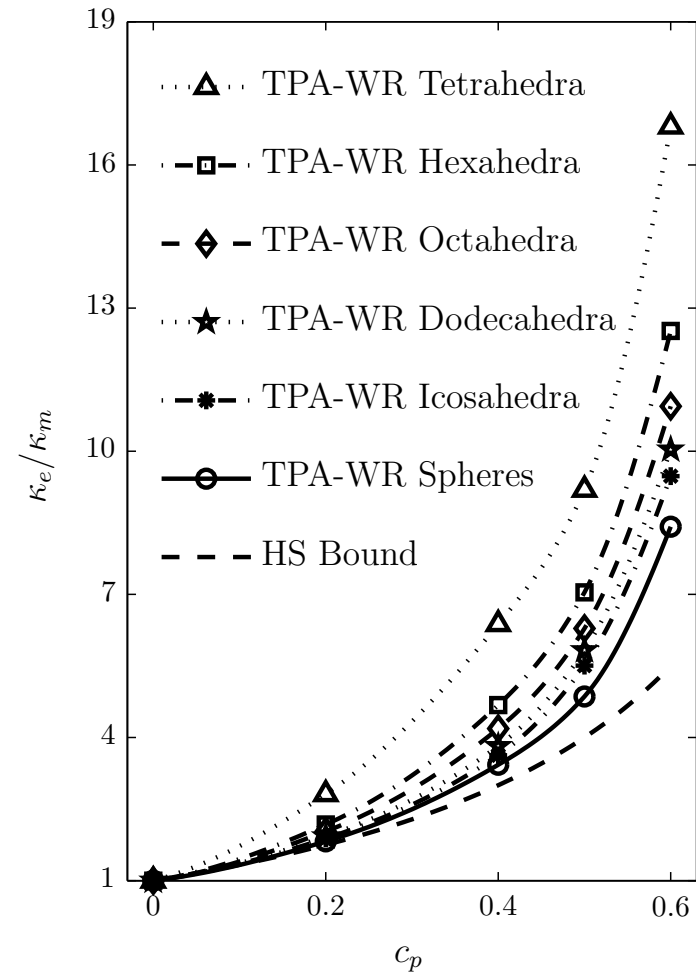
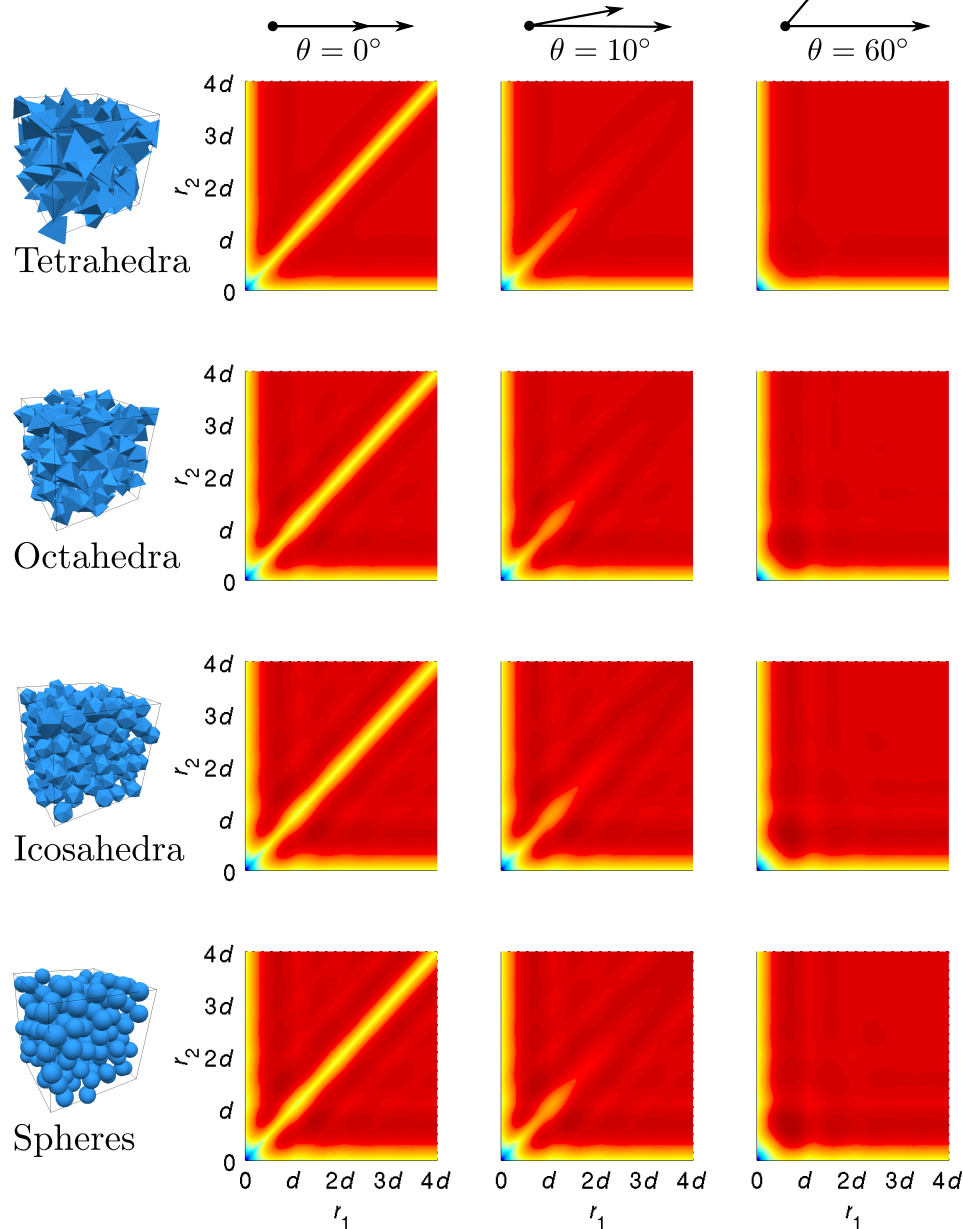
- Image-driven modeling - Representative Unit Cell (RUC)
- Shock thickness $\sim 1\text{-}5$ particle diameters
- Need to resolve sub-crystal levels - $\sim 0.02 \text{ } \mu\text{m}$

► Continuum modeling concept

Computational Physics Highlights

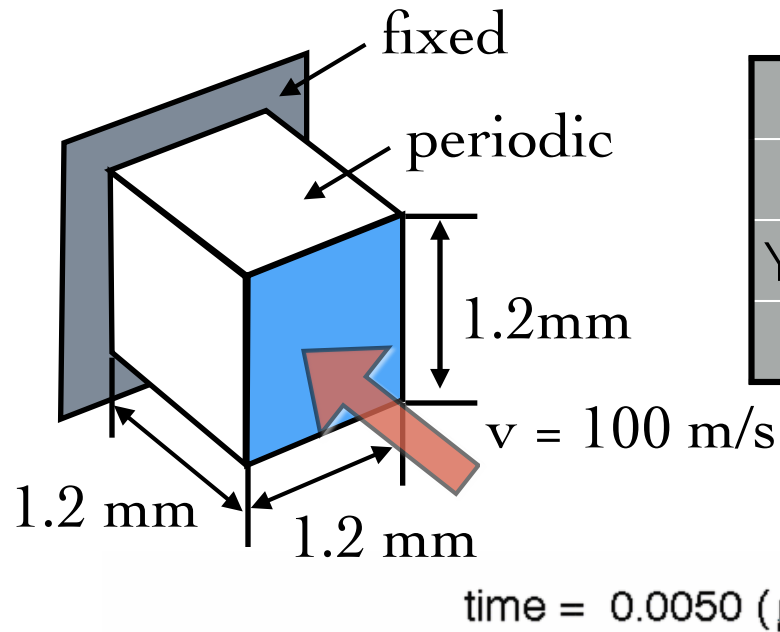
- Image-Based Statistical Modeling of Polydisperse Media
- Shock Simulations in Heterogeneous Solids
- Hierarchically Parallel Computational Homogenization
- Asynchronous Multi-Domain Space-Time Integrators
- Lagrangian Eulerian Coupling
- Wavelet Adaptive Multiresolution Resolution Solver

Image-Based Modeling, Shape Effect



Third-order Statistical Micromechanics ► LANL Mustang, 7200 cores

Shock Simulations in Heterogeneous Materials

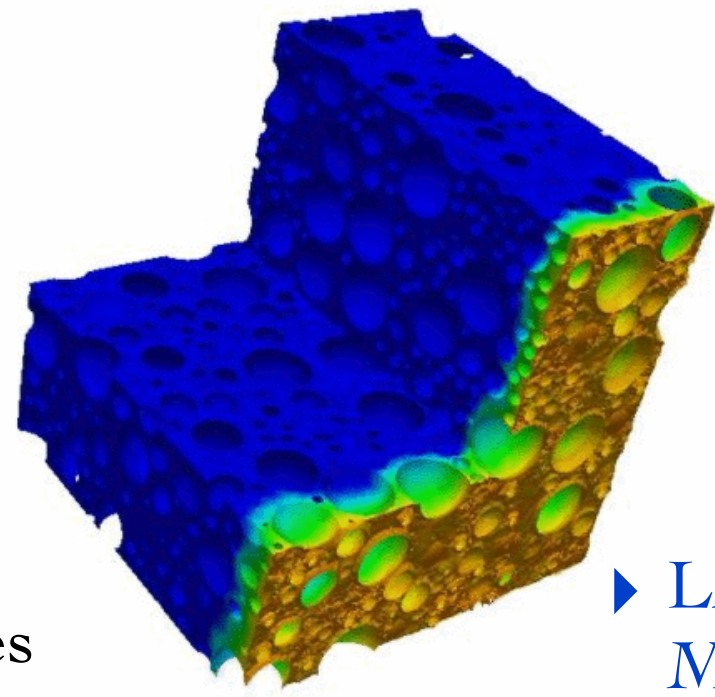
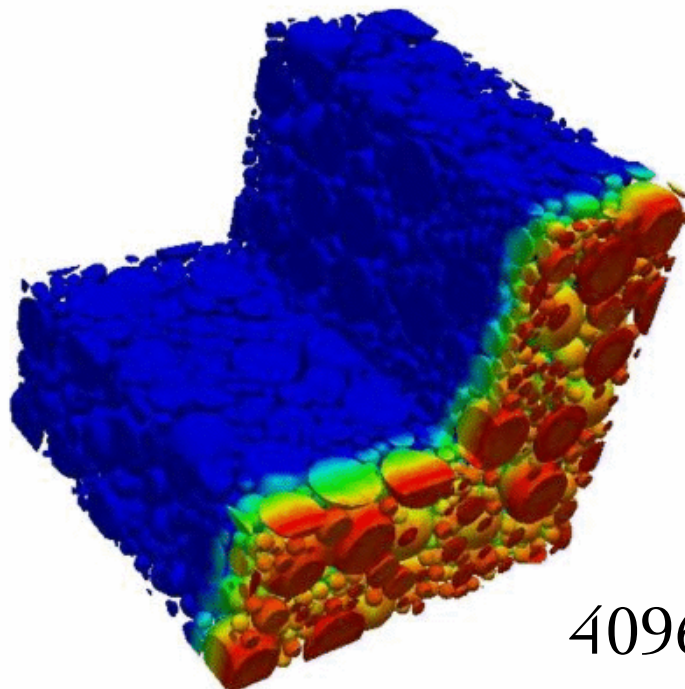
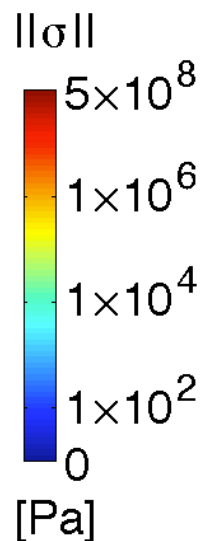


	Ni	Al	Matrix
Particle radius [μm]	100	50 / 25	-
Young's modulus [GPa]	225.9	100	0.1
Density [kg/m ³]	9000	2700	500

Number of elements : 18,227,610

$\Delta t = 0.2 \text{ ns}$, $c_{\text{par}} = 0.7$

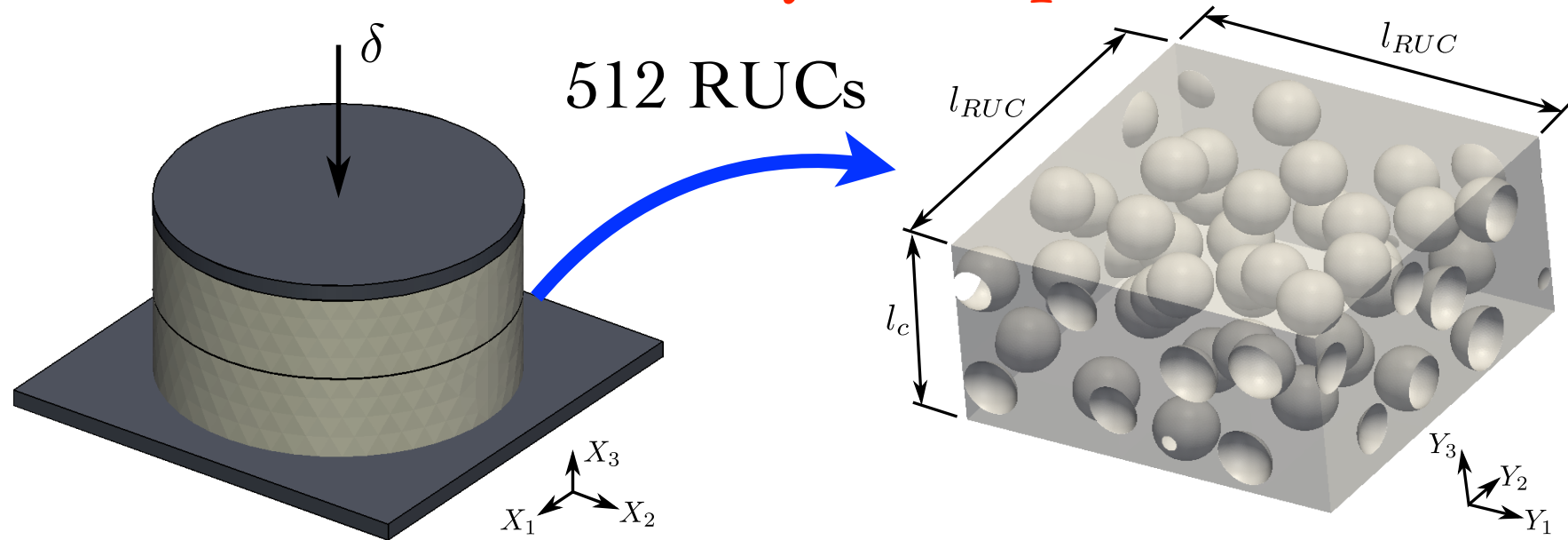
time = 0.0050 ($\mu \text{ sec}$)



► LANL
Mustang

Path towards first year simulations

Reverse Taylor impact



■ Macro-scale

- No-slip on top/bottom
- $h = 10 \text{ mm}$, $d = 20 \text{ mm}$

■ $E = 15 \text{ GPa}$, $\nu = 0.25$

■ 15K elements in Macro

■ Micro-scale

- $250 \times 250 \times 125 \mu\text{m}^3$
- 40 voids, $40 \mu\text{m}$ diameter

■ $E = 5 \text{ GPa}$, $\nu = 0.34$

■ 5M elements in RUC

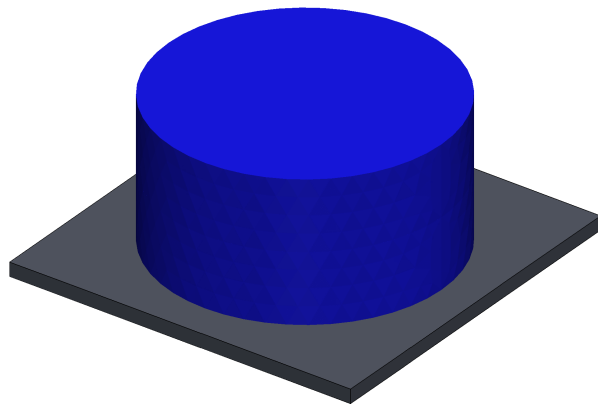
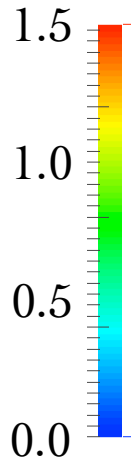
► Quasi-steady loading conditions, Nonlinear hyper-elasticity

Multi-scale Simulations, *PGFem3D* - GCTH

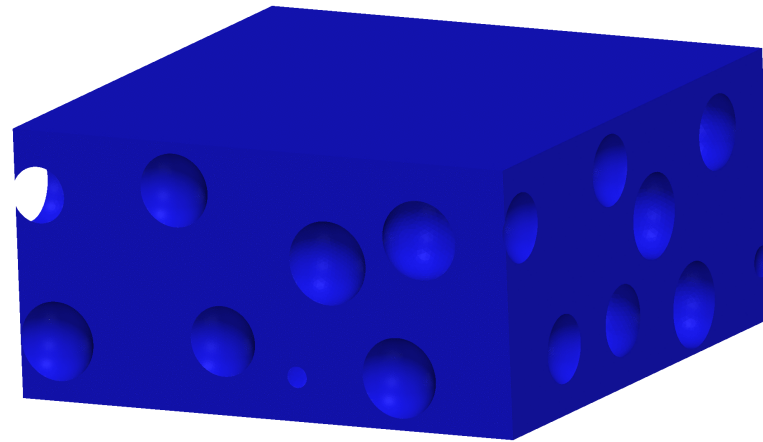
■ 487M Node, 2.65B Elements, 1.39B DOF, 64K cores

► LLNL Vulcan

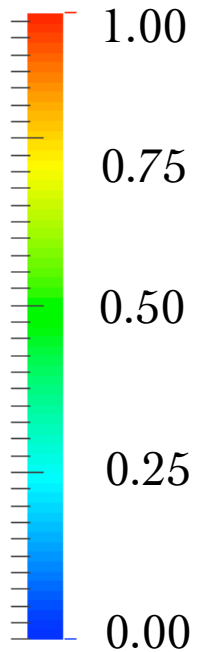
$\|\sigma\|$ GPa



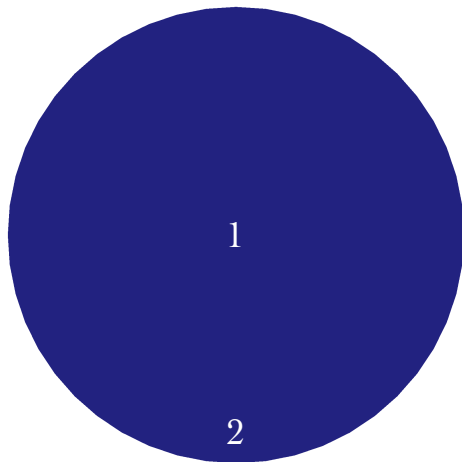
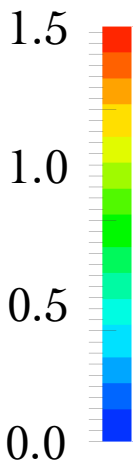
1



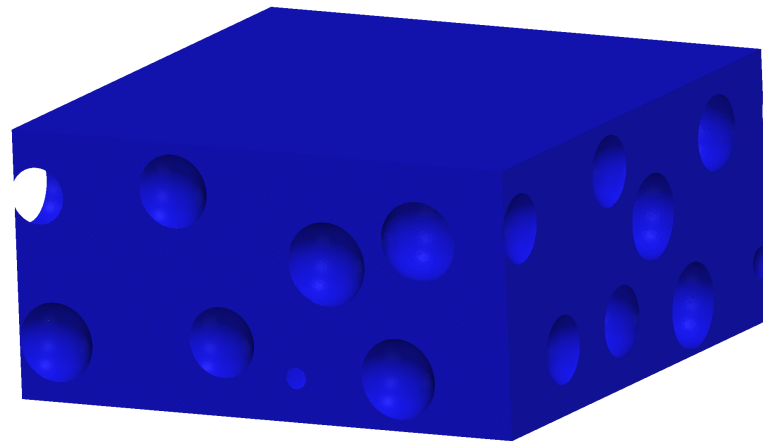
$\|e\|$



$\|t\|$ GPa



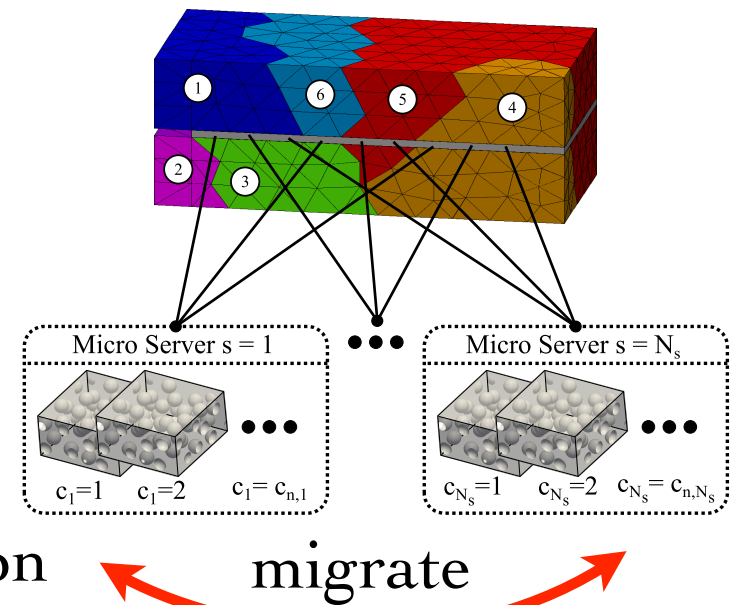
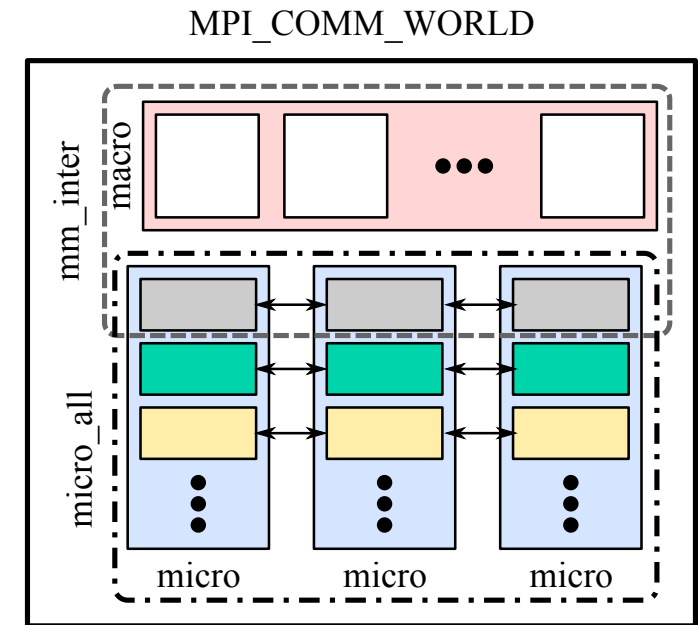
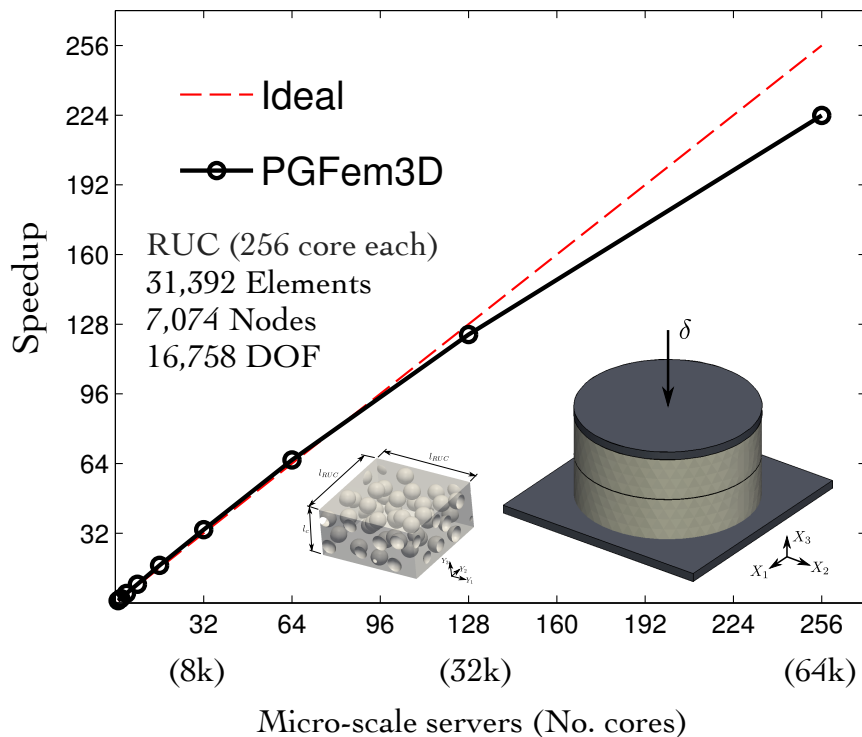
2



512 RUCs

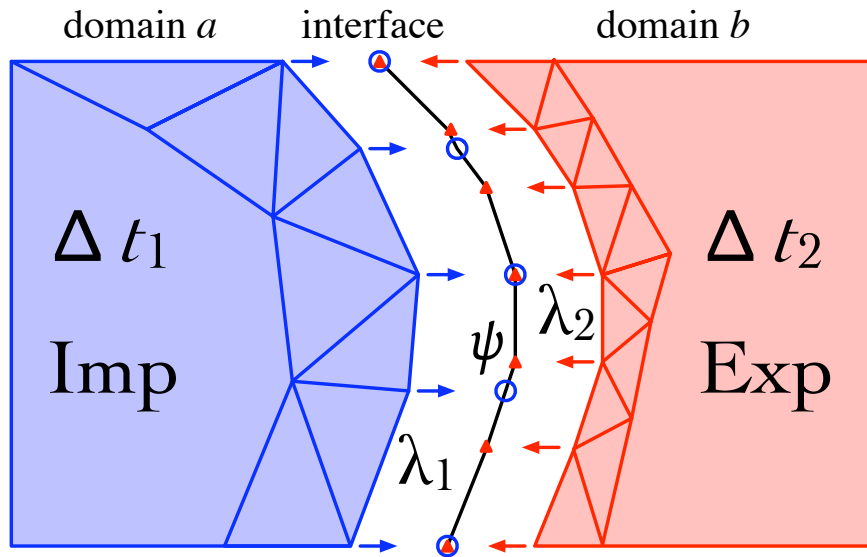
$h_e(\text{min}) = 60 \text{ nm}$

Multi-scale Simulations, *PGFem_{3D}* - GCTH



- Load-balancing for microscale simulations
 - Time-based metrics for adaptation, heuristics
 - Non-blocking data migration among servers/computing nodes
 - Overlay computations with data migration

Asynchronous Multi-Domain Space-Time Integrators



- Energy, momentum preserving
- Space-time discontinuous
- Mixed integration natural
- Second order accurate
- Highly parallel

- Equation of motion

$$\rho_0 \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla_0 \cdot \mathbf{P} + \mathbf{f}_0$$

- Semi-discrete system of equations

$$\mathbf{M}_s \ddot{\mathbf{u}}_s + \mathbf{K}_s \mathbf{u}_s + \mathbf{R}_s^T \lambda_s = \mathbf{f}_s,$$

$$\mathbf{L}_s \mathbf{u}_s - \mathbf{B}_s \Psi = 0,$$

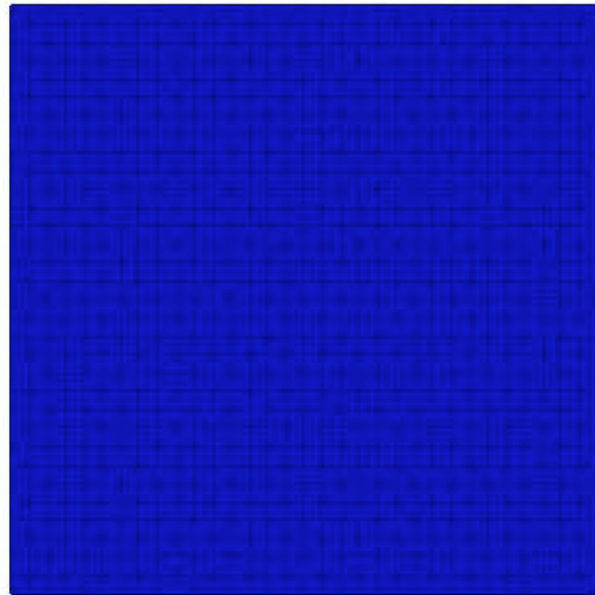
- Reduced, interface system

$$\sum_{s=1}^{n_s} \mathbb{B}^T \mathcal{S}_s \mathbb{B} \Psi = \sum_{s=1}^{n_s} \mathbb{B}^T \mathcal{F}_s$$

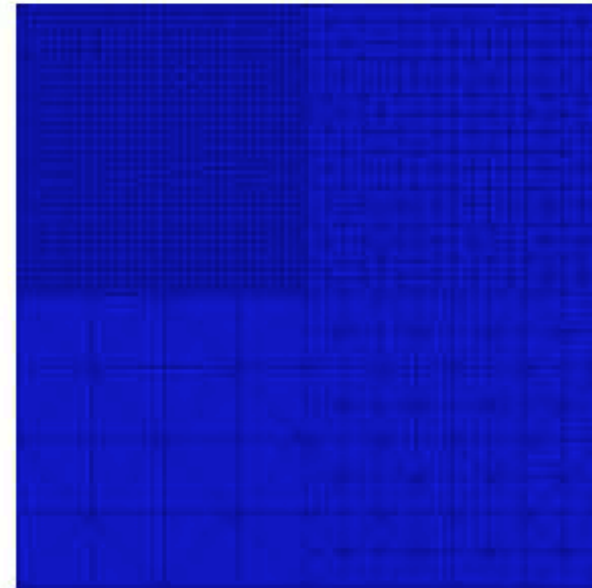
$$\sum_{s=1}^{n_s} -\mathbf{B}_s^T \lambda_s = 0.$$

► Parallel Asynchronous Space-Time Algorithm using a Domain Decomposition Method (PASTA-DDM) with non-matching grids

PASTA-DDM



Time: 1.00

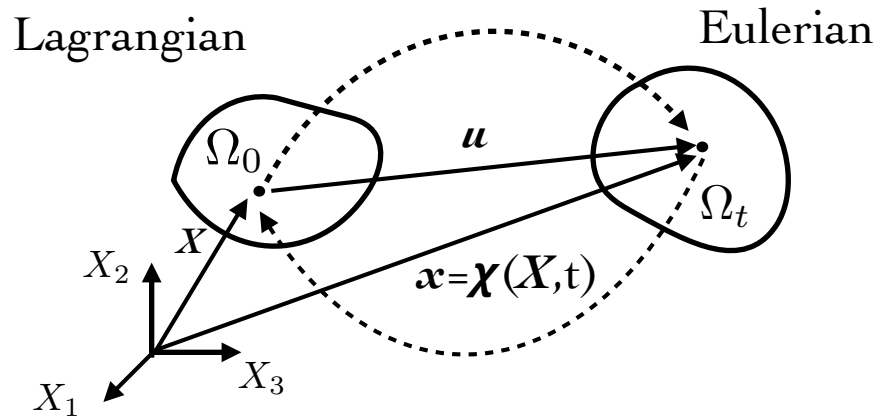


Time: 1.00

Subdomain	Ω	Ω	Ω	Ω
Mesh size	$1/h$	$4/h$	$16/h$	$64/h$
Time step	Δt	$2\Delta t$	$3\Delta t$	$4\Delta t$

Lagrangian Eulerian Compatibility (LEC) Condition

$$\chi(\mathbf{X}, t) : \Omega_{M_0} \rightarrow \Omega_M \in \mathbb{R}^3$$



$$\mathbf{F}(\mathbf{X}, t) = \frac{\partial \chi}{\partial \mathbf{X}}, \quad \mathbf{f} = \mathbf{F}^{-1}, \quad \mathbf{l} = \nabla \mathbf{v}$$

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{V}(\mathbf{X}, t) = \frac{\partial \chi}{\partial t}$$

■ Manufactured solution

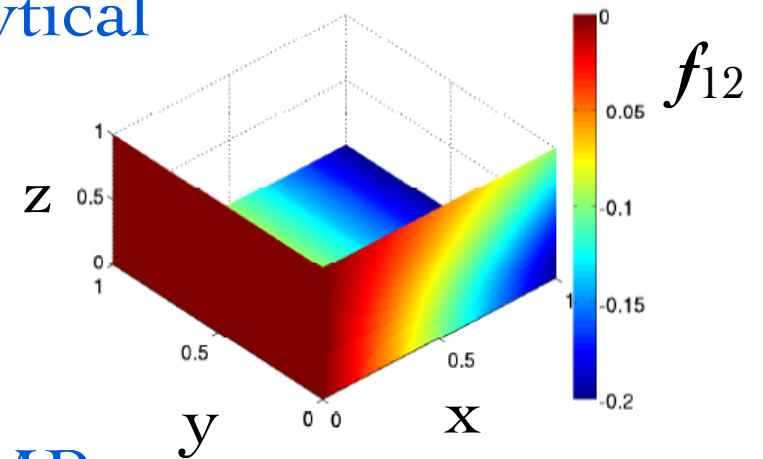
$$\Omega \in [0, 1]^3 \quad v_1 = \frac{7t^6(1 + x_2^2)}{10(1 + x_3^2)}$$

$$v_2 = 0, \quad v_3 = 0$$

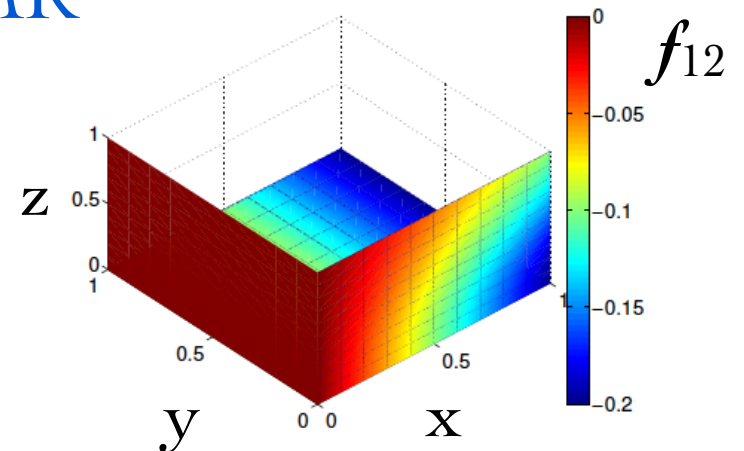
$$\dot{\mathbf{F}} = \mathbf{l}\mathbf{F}, \quad \dot{\mathbf{f}} = -\mathbf{f}\mathbf{l}$$

$$\frac{\partial \mathbf{f}}{\partial t} + \nabla \mathbf{f} \mathbf{v} + \mathbf{f} \nabla \mathbf{v} = 0$$

► Analytical



► WAMR



3D Macro-scale simulation, *WAMR*

- Domain

$[0, 3] \times [0, 0.4] \times [0, 0.4]$ cm

- Ambient Mixture

$Y_{N_2}=0.868$, $Y_{O_2}=0.232$

$P=101.3$ kPa

$T=1000$ K

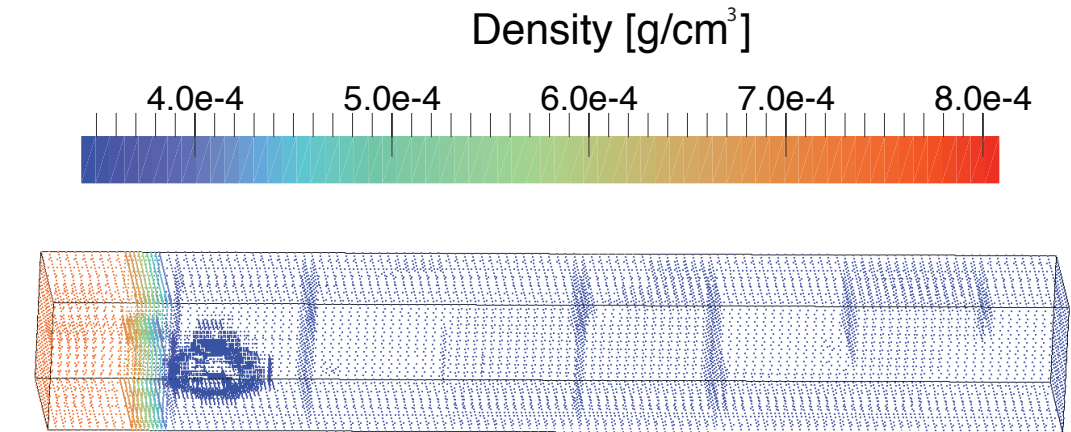
- Bubble

$Y_{H_2}=0.990$

$r=0.1$ cm at $x=0.5$ cm

- Loaded by Shock

$M_s = 1.5$ at $x=0.3$ cm



- Wavelet parameter

$\epsilon=10^{-2}$

$p=4$

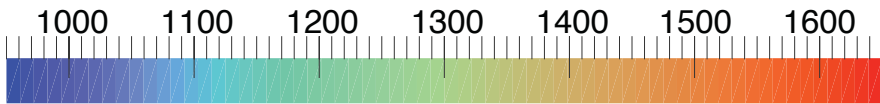
$[N_x \times N_y \times N_z]_{\text{coarse}}=[60 \times 8 \times 8]$

- Reactive mixture

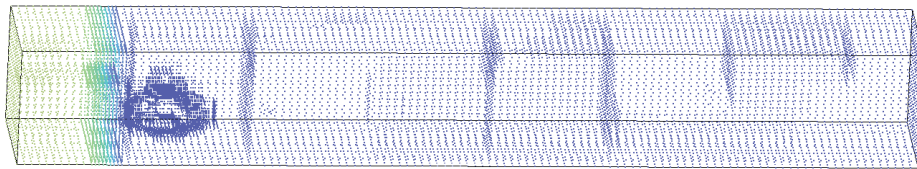
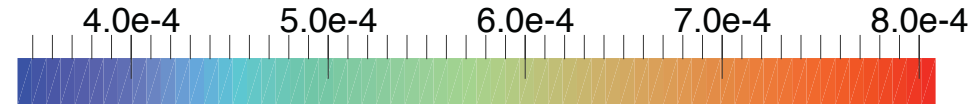
9 species, 19 reactions

3D Macro-scale simulation, *WAMR*

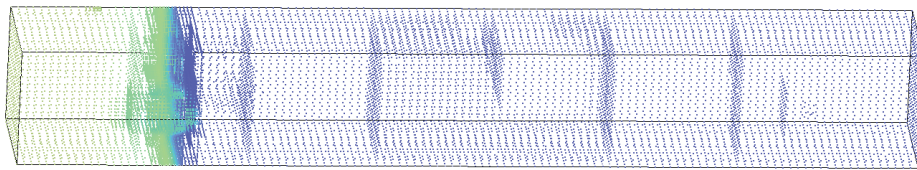
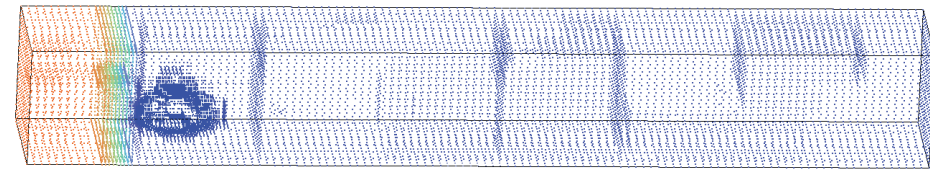
Temperature [K]



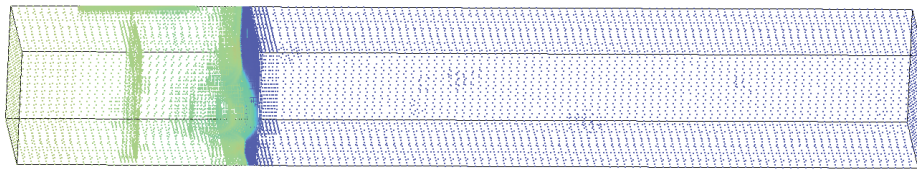
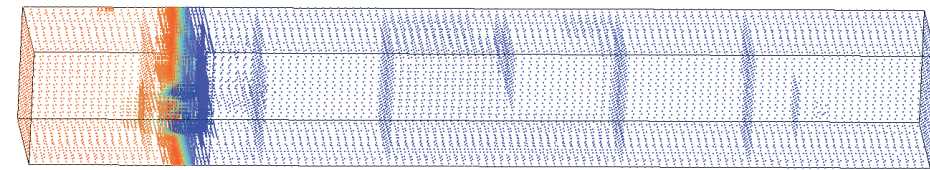
Density [g/cm³]



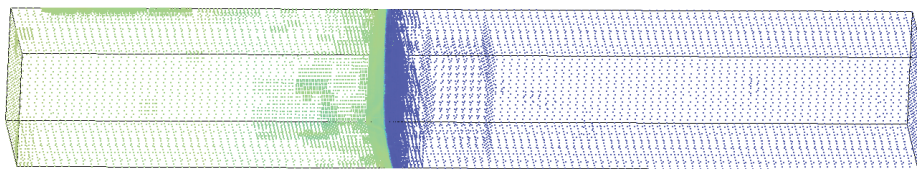
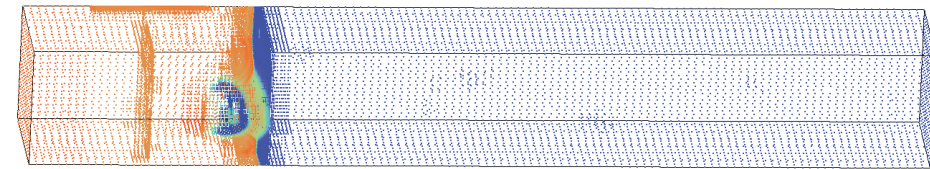
0 μs



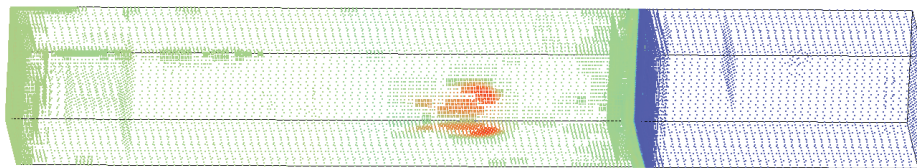
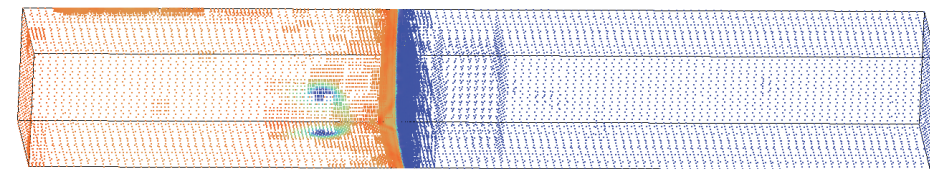
2.5 μs



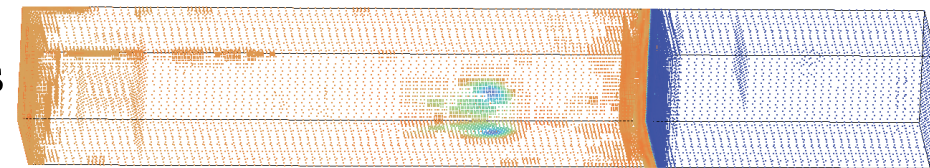
5 μs



10 μs



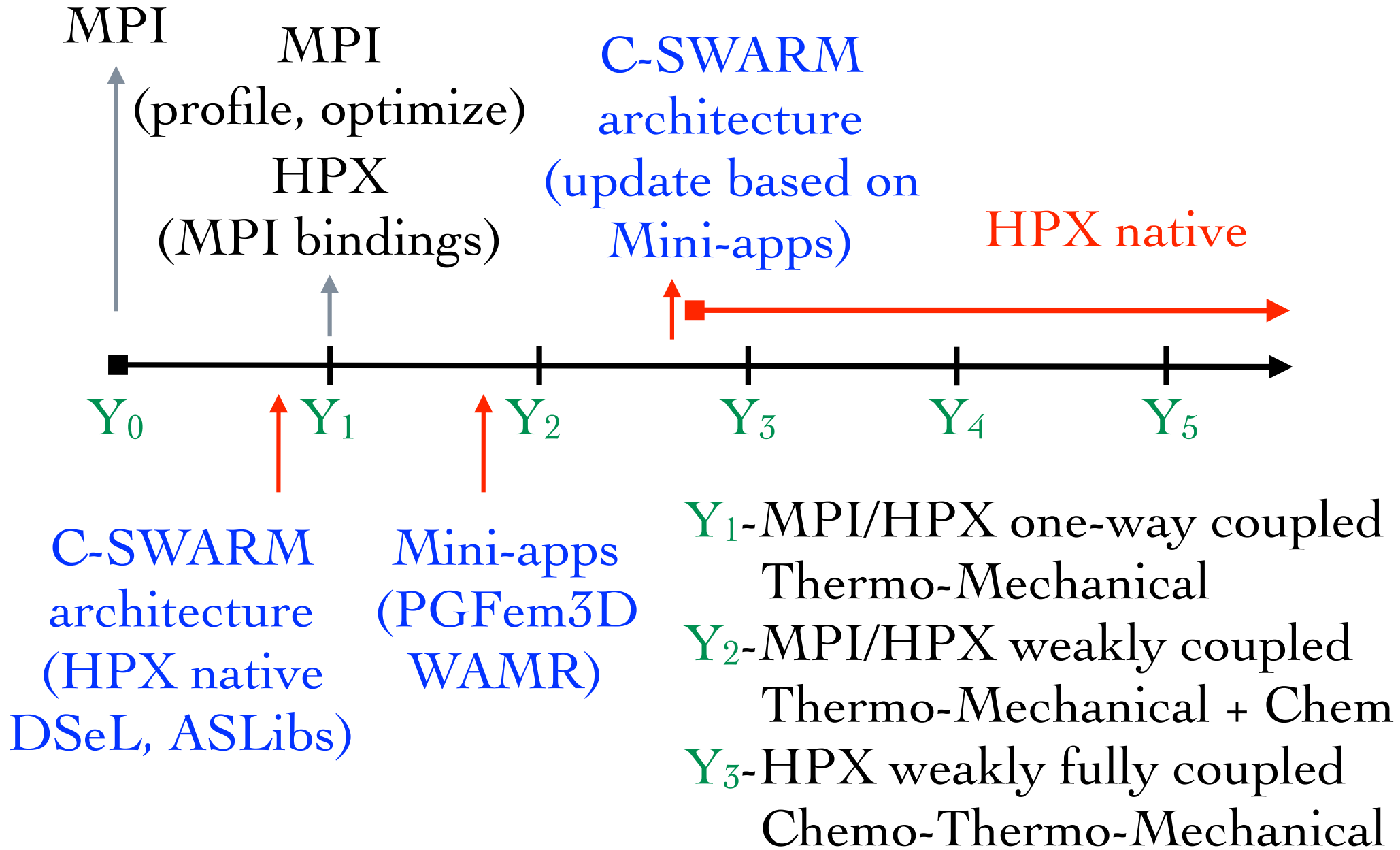
18.75 μs



Computer Science Highlights

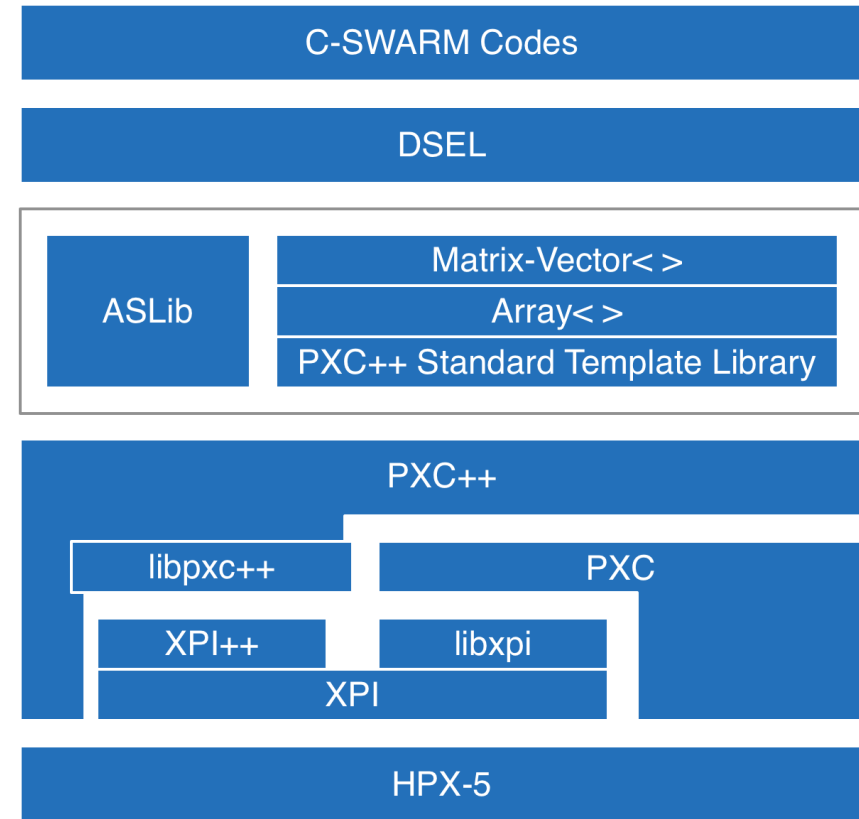
- Develop software infrastructure to make C-SWARM applications possible on current and next-generation (Exascale) HPC platforms
- New HPX advancements
- Mini-apps
- Separate science from details of runtime system, computer architecture via domain-specific language and libraries (DSL), advanced software libraries (ASLib), and run-time interfaces (XPI)

CP/CS and SP Integration



Software Stack

- Codes will be implemented in domain-specific language and libraries (DSL)
- DSL will source-to-source compile to PXC++
- STL and common data structures will be implemented in PXC++
- PXC++ exposes XPI semantics and runs on top of HPX-5
- HPX-5 manages system resources for PXC++



HPX Development

- HPX run-time system manages resources for parallel computational science applications
- Completed the development of a stable HPX runtime system that expanded the number of available types of LCOs
- Implemented two different global address spaces (partitioned and active) which support distributed memory operations for applications
- Developed several mini-apps (WAMR-HPX, Heat Equation-HPX, PASTA-DDM-HPX) on stabilized runtime system

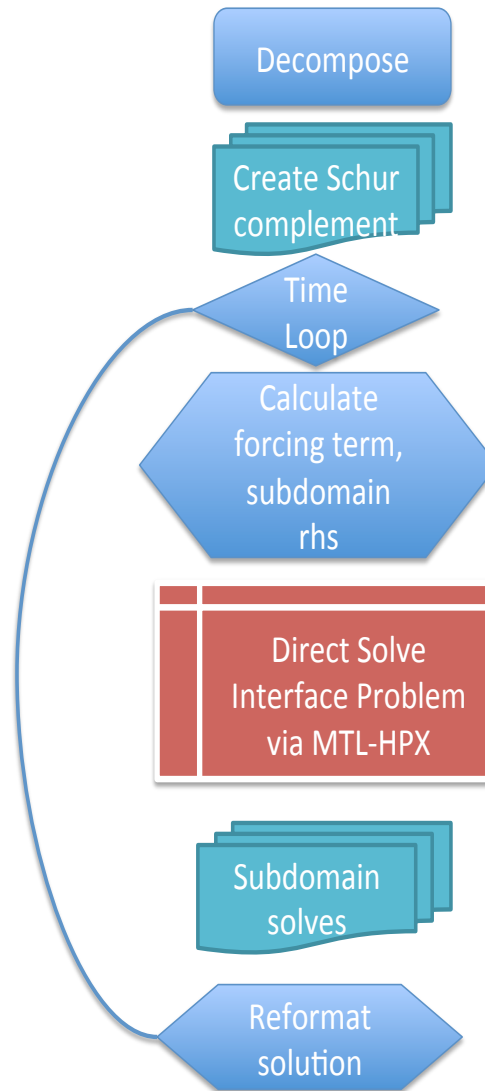
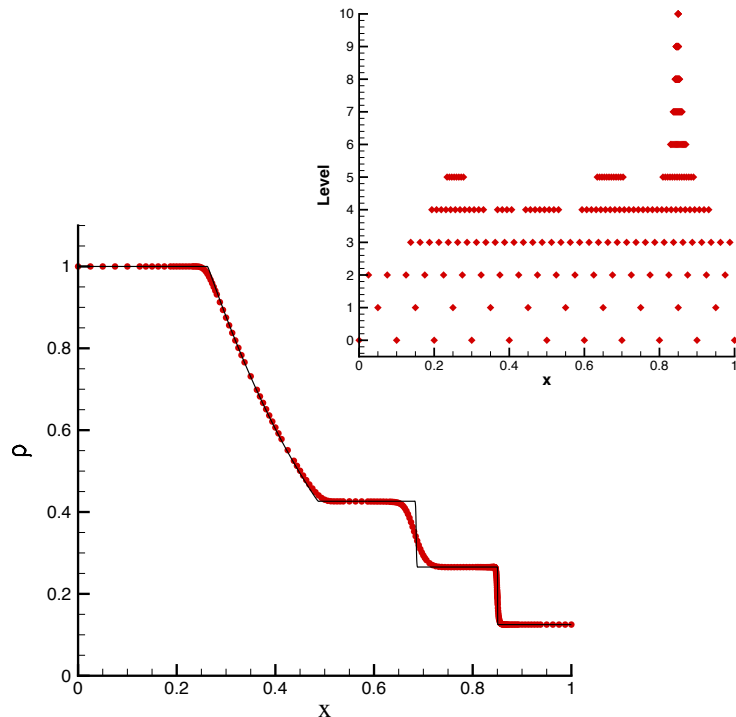
Mini-apps, WAMR-HPX and PASTA-DDM-HPX

Testing: Sod problem

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p - \tau)}{\partial x} = 0$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial((\rho E + p)u - u\tau + q)}{\partial x} = 0$$



- Matlab mini-app of PASTA-DDM complete
- Redesign of Matlab mini-app for use with HPX
- Initial design work replacing Matlab with MTL and HPX
- PASTA-DDM will be implemented using

Mini-apps, Heat Equation - HPX

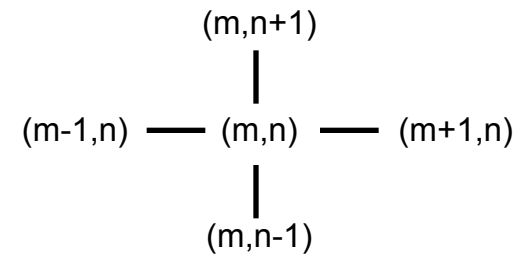
$$\frac{\partial T}{\partial t} = \nabla \cdot (\nabla T)$$

$$T(\mathbf{x}, t_0 = 0) = \sin(\pi x_1) \sin(\pi x_2) \quad \text{in } \Omega$$

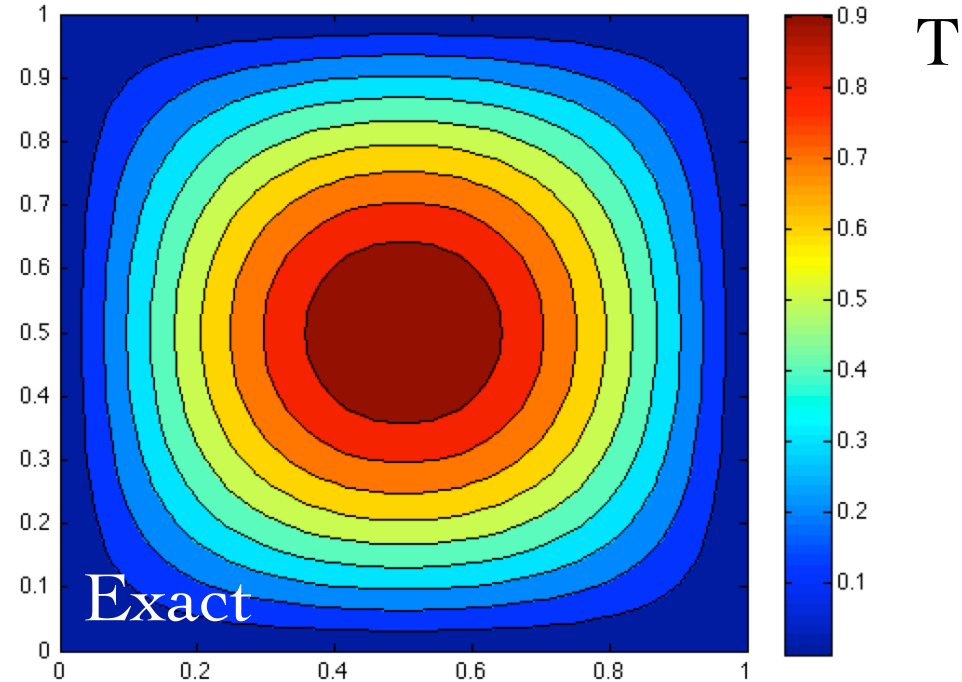
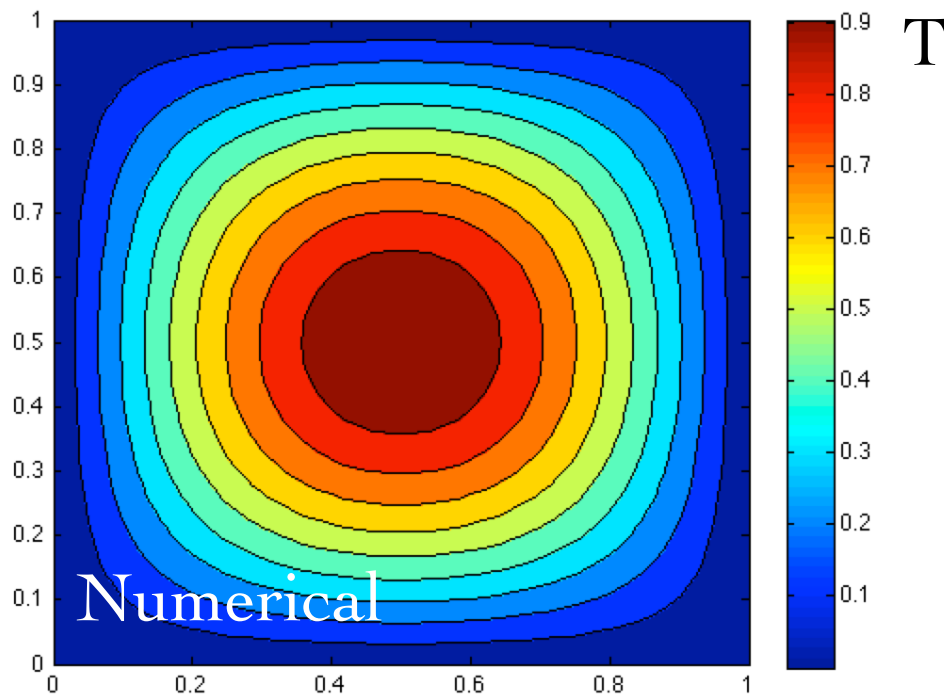
$$T = 0 \quad \text{on } \partial\Omega$$

$$T(\mathbf{x}, t) = e^{-2\pi^2 t} \sin(\pi x_1) \sin(\pi x_2)$$

connectivity



$$T_{m,n}^{k+1} = T_{m,n}^k + \Delta t \frac{T_{m,n+1}^k + T_{m,n-1}^k + T_{m+1,n}^k + T_{m-1,n}^k - 4T_{m,n}^k}{h^2}$$



Mini-apps, Heat Equation - HPX

```
static int action_integration(ArgIntegrate *arg){
    hpx_addr_t local = hpx_thread_current_target();
    Domain *ld = NULL;
    if (!hpx_gas_try_pin(local, (void**)&ld))
        return HPX_RESEND;
```

global memory pinned
prior to reading/writing

```
if(value->IsItMe) {
    ld->T += (1.0 - dt*4.0/h/h)*ld->Tn;
```

contribution to itself

```
new_arg.IsItMe = false;
new_arg.value = (dt/h/h)*(ld->Tn);
hpx_addr_t done = hpx_lco_and_new(itgno);
for(int a = 0; a<4; a++){
    hpx_addr_t block = hpx_addr_add(ld->D,
        sizeof(Domain)*ld->Gid[a+1], sizeof(Domain));
    hpx_call(block, integration, &new_arg, sizeof(new_arg), done);
}
hpx_lco_wait(done);
hpx_lco_delete(done, HPX_NULL);
```

send data to the neighbors

```
else
    ld->T += arg->value;
```

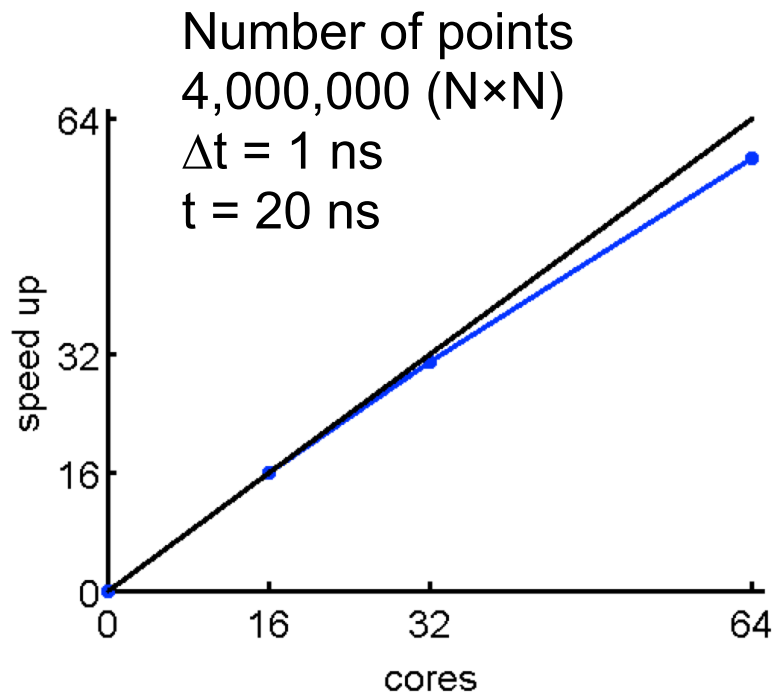
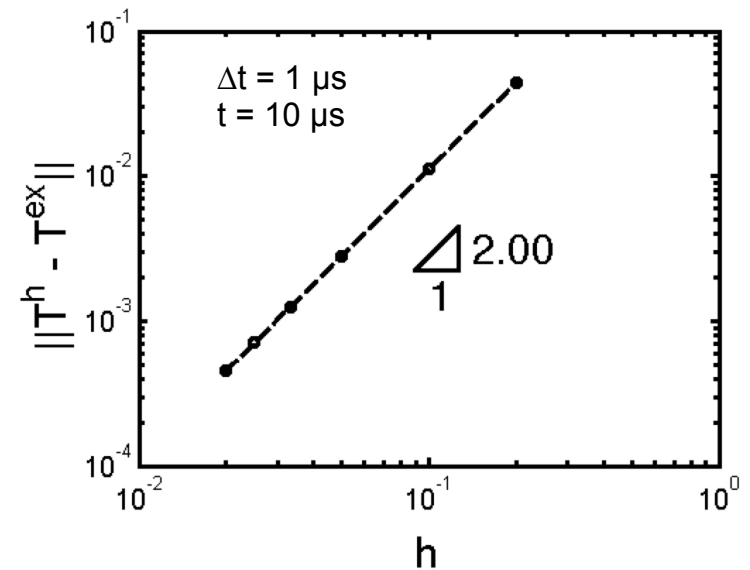
integrate data from neighbors

Global Address Space – Allocation

```
int hpx_heat_eq_main(const main_args_t *args){
    hpx_addr_t domain = hpx_gas_global_alloc(nDom, sizeof(Domain));
```

```
for (int a = 0; a < nDom; a++){
    arg.IsItMe = true; arg.value = 0.0;
    hpx_addr_t block = hpx_addr_add(domain, sizeof(Domain)*a, sizeof(Domain));
    hpx_call(block, integration, &arg, sizeof(arg), complete);
}
hpx_lco_wait(complete);
hpx_lco_delete(complete, HPX_NULL);
```

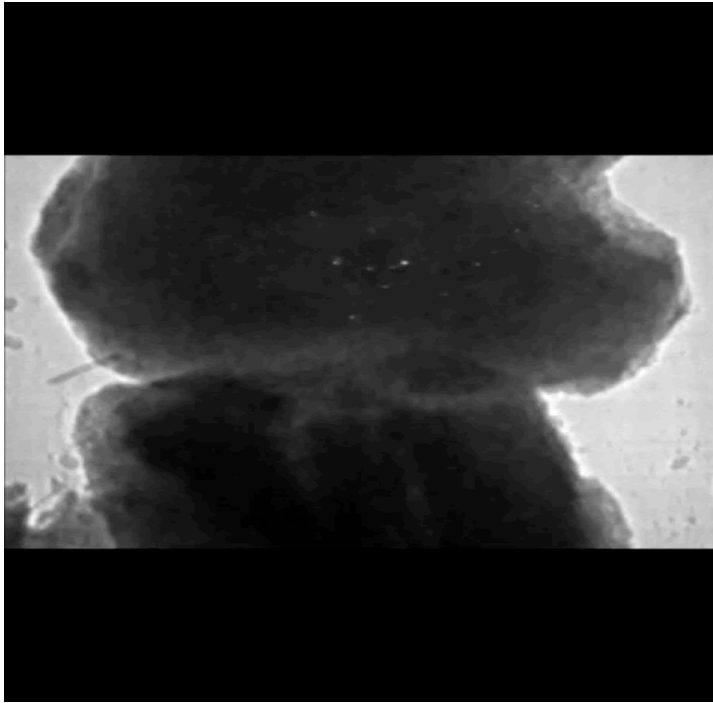
integration loop



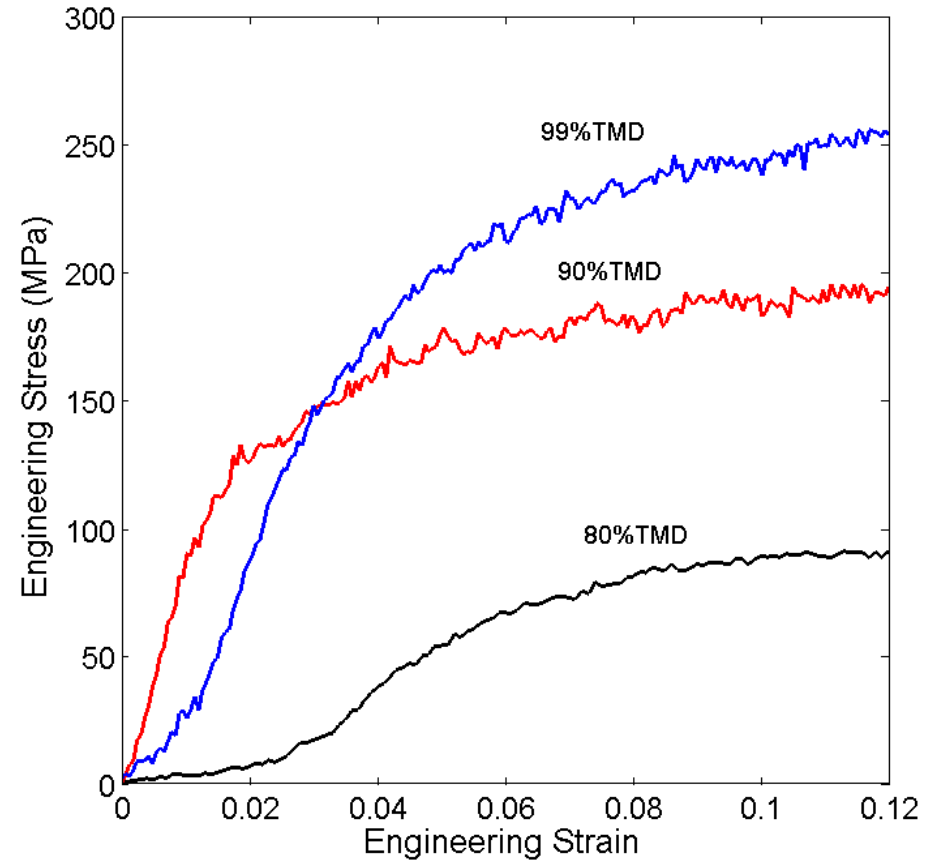
V&V/UQ Experimental Physics Highlights

- Provide Verification Platform
- Material Characterization
- Calibration Experiments
- Validation Experiments
- Uncertainty Quantification

Calibration Experiments



- Two particle interaction, Ni/Al
- Particle size $355 < d < 850 \mu\text{m}$
- Crack propagation observed in particle on the bottom

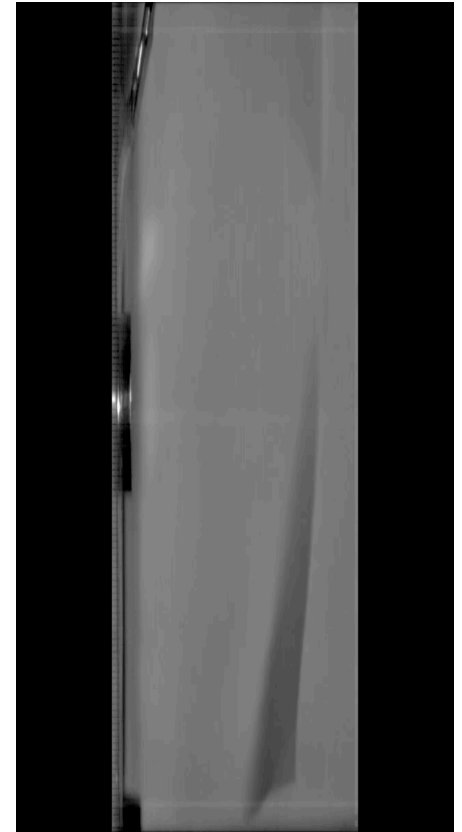


Kolsky bar (Al)

- Calibrate thermo-mechanical properties at finest scale
- Use inverse analysis and Bayesian framework to calibrate variables from microscale

Validation: Hierarchy of Experiments

- Micro: quasi-steady properties at the RUC level, conductivity, dynamic elasto-viscoplastic properties; post-mortem characterization of final morphology.
- Micro-macro: Asay shear impact, to be described, allows viewing of thermal response, ignition, and local surface strain field in response to impact; quasi-2D
- Macro: full 3D reversed Taylor impact, allows i) strain under dynamical loading, ii) initiation threshold and resulting reaction propagation via impact experiments, and iii) properties of the resulting synthesized material. **Embodies all scales.**



The original Taylor test fired long cylinders at a solid backstop, our arrangement uses a fixed cylinder impacted by a flyer plate.

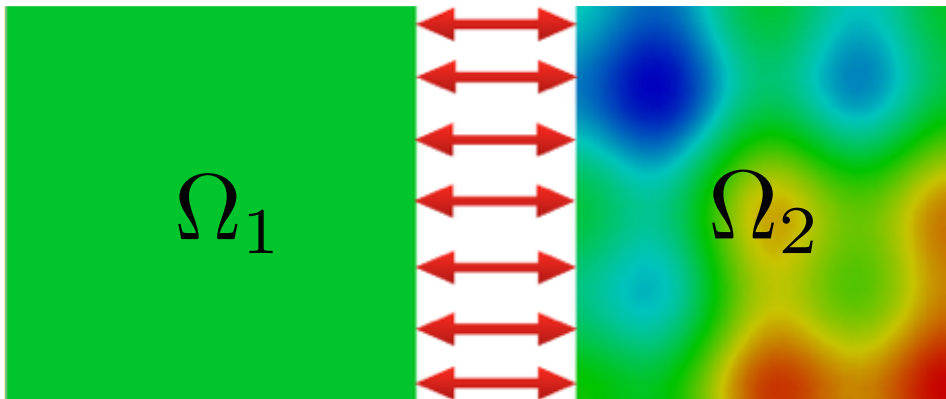
UQ

► Our computational framework is based on the Design Analysis Kit for Optimization and Terascale Application (DAKOTA) from Sandia National Laboratories

- Uncertainty quantification
- Parameter estimation
- Sensitivity analysis
- Design and analysis of computer experiments (DACE)
- Reliability analysis
- Bayesian calibration

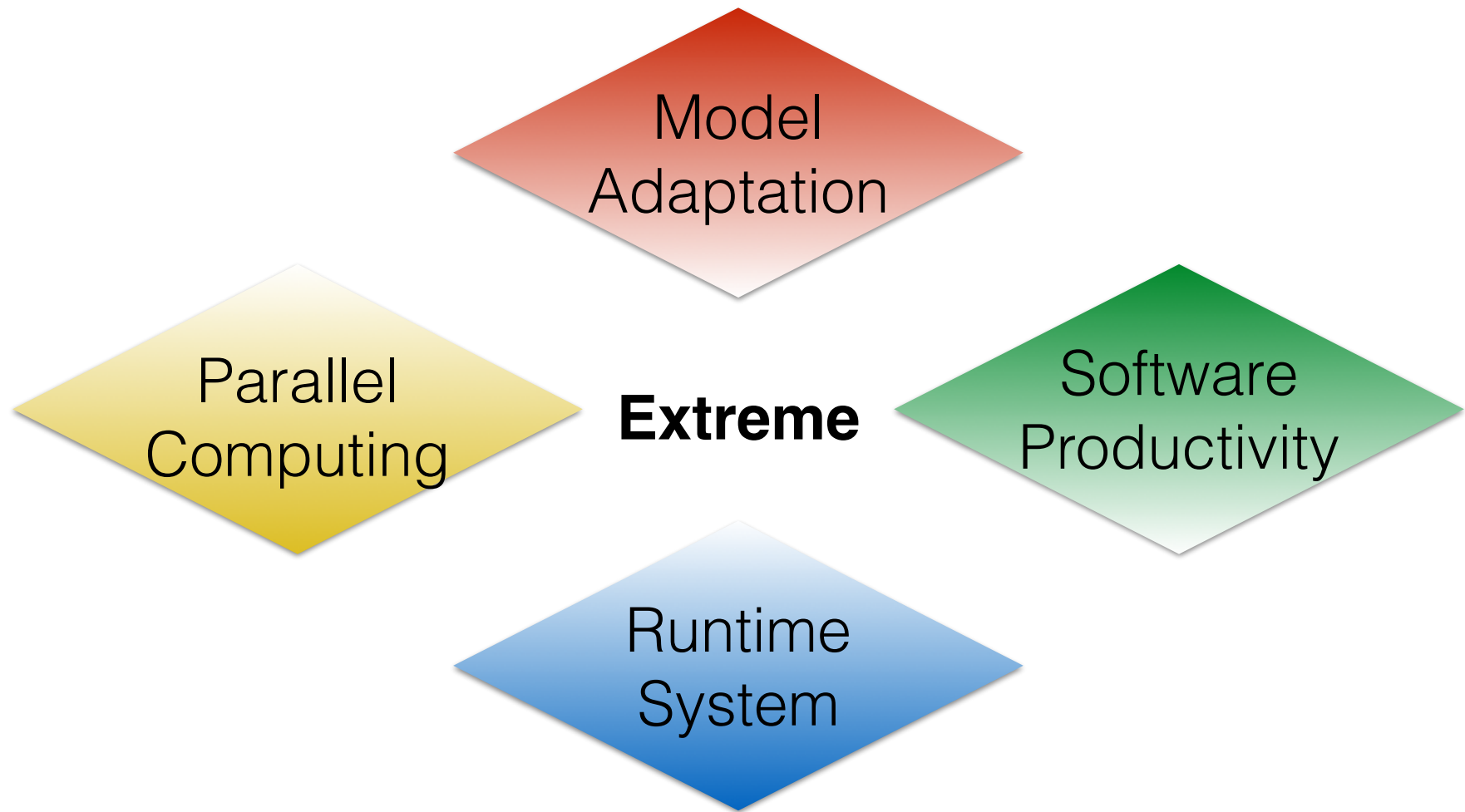


■ Concept of localized uncertainty



- Synergy between CP, EP and CS
- PASTA-DDM

Extreme Scale Computing Workshop



March 2-3, 2015, Bloomington, IN.

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